

**Synthesis, Structural investigations and Properties of a  
few Transition Metal Supramolecular Coordination  
Solids involving N- and O-Donor Ligands**



**Thesis**

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*Submitted by*

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## 5.4 CONCLUSIONS

Three new pyridine based coordination compounds of Co(II), Ni(II) and Cu(II) *viz.* [Co(py)(2,6-PDC)(H<sub>2</sub>O)<sub>2</sub>] $\cdot$ H<sub>2</sub>O (**10**), [Ni(py)(2,6-PDC)(H<sub>2</sub>O)<sub>2</sub>] $\cdot$ H<sub>2</sub>O (**11**) and [Cu(py)(2,6-PDC)(H<sub>2</sub>O)] $\cdot$ 2H<sub>2</sub>O (**12**) have been synthesized and characterized by single crystal X-ray diffraction, electronic, vibrational spectroscopy and thermogravimetric analysis. The isostructural complexes **10** and **11** are further characterized by PXRD and their isostructurality parameters are evaluated by using Fabian and Kalman approach. Several non-covalent interactions including the antiparallel  $\pi$ -stacking interactions stabilize the layered assemblies in the structures. We have evaluated the strength of the antiparallel  $\pi$ -stacking interactions and the influence of the pyridine coordination to the strength of the stacking assembly using DFT calculations. The dimerization energy of the self-assembled dimer in the layered architecture is larger for complex **12** due to the participation of C–H $\cdots$ O hydrogen bonds involving the carboxylate groups. The antiparallel  $\pi$ -stacking and C–H $\cdots$ O interactions have been characterized by using the NCI plot index, which is in good agreement with the energetic and MEP results. All the three complexes significantly inhibit cell viability by inducing apoptotic cell death in cancer cell line with negligible cytotoxicity in normal cells. Interestingly, the molecular docking study reflects that the complexes **10**, **11** and **12** interact and accommodated well in the active sites of anti-apoptotic protein BCL-2 that might lead to apoptotic cell death. Furthermore, the pharmacophore features embedded with the synthesized complexes may play important role during biological activities.

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